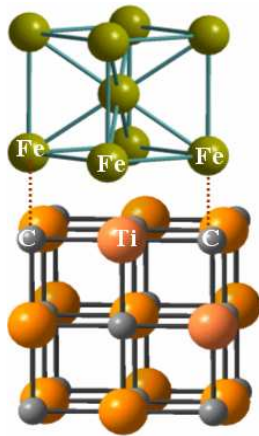


MULTI-SCALE MODELING AND ANALYSIS FOR DESIGN OF ADVANCED STEELS

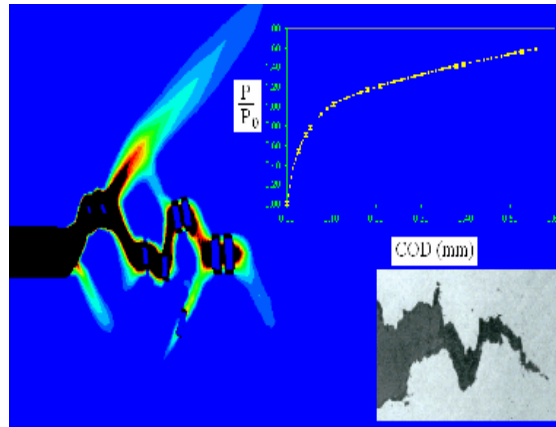
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Strength and fracture toughness are the primary property-indices for steels. Combining these two conflicting properties motivates this ONR-funded project at Northwestern University focused on the multiscale/quantum design of new “triple-phase” high toughness plate steels for blast resistant applications. In order to establish the relationships among alloys selection, heat treatment process, micro/nano-structural parameters and ductile fracture toughness, a computation-based hierarchical material design model is developed that links mechanisms at the quantum scale by considering the inclusion/iron matrix interfacial debonding within a two-level (micro and sub-micro) cell models incorporating the plastic deformation induced phase transformation in the iron matrix for the prediction of fracture toughness [1-9].



Interfacial separation at atomic scale



Debunding-voids coaleasence
induced ductile crack growth

References

- [1] G. B. Olson, "Computational design of hierarchically structured materials." *Science* 277(5330), p. 1237-1242, 1997.
- [2] H. Krakauer and A. J. Freeman, "Linearized Augmented Plane-Wave Method for the Electronic Band-Structure of Thin-Films.", *Physical Review B* v. 19(4), p. 1706-1719, 1979.
- [3] Socarate, S. and D. M. Parks. 1995, MIT: Cambridge, MA.
- [4] A. Needleman, "A continuum model for void nucleation by inclusion debonding", *J. Appl. Mech.*, v. 54(3), p. 525-531, 1987.
- [5] J. R. Rice and M. A. Johnson, "The Role of Large Crack Tip Geometry Changes in Plane Strain Fracture", in *Inelastic Behavior of Solids* (eds. M. F. Kanninen, et al.), McGraw-Hill, N.Y., 1970, pp. 641-672.
- [6] Gao, H., Huang, Y., Nix, W.D., and Hutchinson, J.W., *Mechanism-based strain gradient plasticity - I. Theory*. *Journal of the Mechanics and Physics of Solids*, 1999. **47**(6): p. 1239-1263.
- [7] Hughes, T.J.R., *Multiscale Phenomena - Greens-Functions, the Dirichlet-to-Neumann Formulation, Subgrid Scale Models, Bubbles and the Origins of Stabilized Methods*. *Computer Methods in Applied Mechanics and Engineering*, 1995. **127**(1-4): p. 387-401.
- [8] Liu, W.K., Hao, S., Belytschko, T., Li, S. F., Chang, C. T., *Multiple scale meshfree methods for damage fracture and localization*. *Computational Materials Science*, 1999. **16**(1-4): p. 197-20
- [9] Hao, S., W. K. Liu, C. T. Chang (2000), *Comp. Methods in Appl. Mech. Engr.* **187**(3-4): 401.